Comments and Addenda

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Random-bond Ising chain in a magnetic field

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The magnetization m as a function of magnetic field h for various temperatures is numerically obtained for the one-dimensional random-bond Ising model with each bond energy either $+J$ or $-J$ with equal probability. For high temperatures ($kT/J \geq 0.6$) the results obtained agree with those of Landau and Blume. We have obtained m vs h for low temperatures as a numerical approach to the zero-temperature limit.

The nearest-neighbor random-bond one-dimensional Ising model, spin-$\frac{1}{2}$, which has been used[1] to model the melting of deoxyribonucleic acid (DNA), has been recently studied by Landau and Blume.[2] The Hamiltonian of the system is given by

$$\mathcal{H}=-J\sum_{i=1}^{N} t_i\sigma_i\sigma_{i+1}-h\sum_{i=1}^{N}\sigma_i \quad , \tag{1}$$

where $\sigma_i=\pm 1$, each t_i equals $+1$ or -1, and $\sum t_i=0$. In the so-called *quenched* case, the *free energy* is averaged over the $N!/[(\frac{1}{2}N)!]^2$ distinct sets of t_i's. In the *annealed* case, on the other hand, the *partition function* is averaged. The problem can be solved analytically in the latter case for arbitrary external field, but not for the quenched case, which is the case treated numerically by Landau and Blume and is the case of interest here.

Whereas in the annealed case one cannot ignore the restriction $\sum t_i=0$,[3] one can do so in the quenched case if $t_i=\pm 1$ with equal probability for each i for reasons that follow. Let $\alpha=N^{-1}\sum t_i$, $\bar{f}(\alpha)$ be the average free energy per spin for a given α, and Ω_α be the number of distinct ways to distribute the $\frac{1}{2}N(1+\alpha)$ positive and $\frac{1}{2}N(1-\alpha)$ negative bonds on an N-bond chain. Then, the average free energy per spin, with no restriction on α, and $t_i=\pm 1$ equally likely, is given by

$$\bar{f}=\frac{1}{2^N}\sum_{\alpha}\Omega_\alpha\bar{f}(\alpha) \quad .$$

Clearly, in the $N\to\infty$ limit, we have

$$\bar{f}=\int\delta(\alpha)\bar{f}(\alpha)\,d\alpha \quad ,$$

which implies $\bar{f}=\bar{f}(\alpha=0)$ if $\bar{f}(\alpha)$ is continuous. We assume it is so, and drop the restriction $\sum t_i=0$ since we will be working with the case $t_i=\pm 1$ with equal probability.

Landau and Blume have calculated (by the Monte Carlo method) the thermal equilibrium values of the magnetization m ($m=N^{-1}\sum_1^N\langle\sigma_i\rangle$) as a function of h, the external field. Their numerical results cover the temperature range $kT/J\geq 0.6$. For such temperatures, m appears to be a smooth function of h.

We have performed numerical calculations on the same system (see below for details) by the transfer-matrix method.[4] For the temperatures covered by Landau and Blume, our results agree with theirs. The results obtained for low temperatures ($kT/J<0.6$) are shown in Fig. 1. In the $T\to 0$ limit, m seems to behave as a discontinuous function of h.

Given $\mathcal{H}$ in (1), the partition function Z for a given set of t_i's is given by

$$Z(\beta J,\beta h;\{t\}_N,N)=Tr\prod_{i=1}^{N}T(t_i) \quad , \tag{2}$$

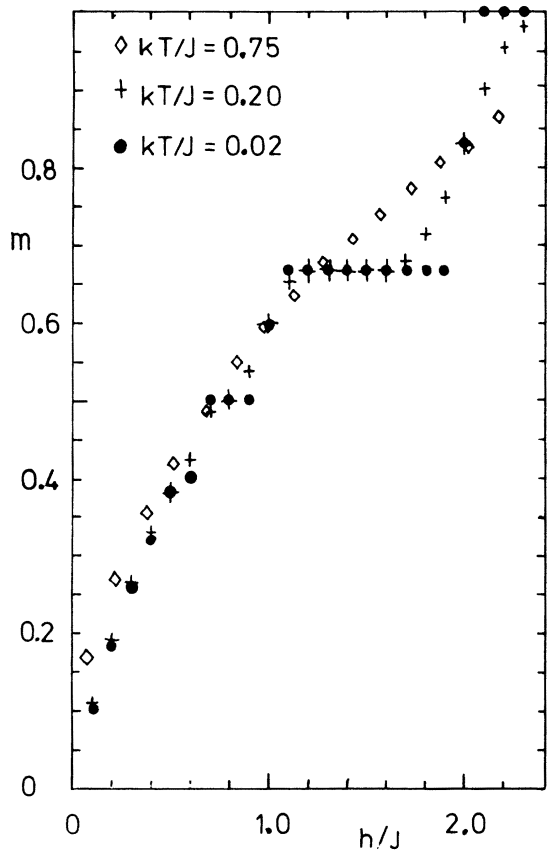

FIG. 1. Low-temperature results of m vs h/J for the values of T shown. The error in the values of m is not larger than 0.01.

where

$$T(t)=\begin{pmatrix}\exp[\beta(tJ+h)] & \exp(-\beta tJ)\\ \exp(-\beta tJ) & \exp[\beta(tJ-h)]\end{pmatrix}, \tag{3}$$

where $\beta=1/kT$, k is Boltzmann's constant, and T is the temperature. The evaluation of Z for the given bond distribution, entails, therefore, carrying out the product of N 2×2 matrices and taking the trace of the result. The expression

$$m'=(N\beta\Delta h)^{-1}[\ln Z(\beta J,\beta(h+\Delta h);\{t\}_N,N) - \ln Z(\beta J,\beta h;\{t\}_N,N)] \tag{4}$$

can be used to obtain the average (over the 2^N different sets of $\{t\}_N$) magnetization m from

$$m=\lim_{N\to\infty}\frac{1}{2^N}\sum_{\{t\}_N}\lim_{\Delta h\to 0} m' \ . \tag{5}$$

The operations indicated in (2) and (4) have been performed for all the values of βJ and βh shown in Fig. 1, with $N=4\times 10^3$, $\beta\Delta h=0.2$, and each t_i chosen at random, with equal weight, to be $+1$ or -1. The operations indicated in (5) were, of course, not performed and therein lies the sources of error in the calculation that shall be discussed below. Each calculation was done for ten randomly chosen sets of t_i's, in order to be able to gauge the error made by not averaging over all the sets of t_i's.

The desired $N\to\infty$ limit of m lies between the maximum and the minimum values of m_{11}, m_{12}, m_{21}, m_{22}, where m_{11} is the magnetization of the finite chain with the two end spins up, m_{12} is the magnetization of the chain with one spin up and the other one down, and so on. The values for m_{11}, m_{12}, m_{21}, m_{22} were calculated for every point in Fig. 1, and bounds on the error δm due to the finiteness of the chain were thus obtained.

The second source of error is due to the fact that the sum $\sum_{\{t\}}$ in Eq. (5) was not performed. Instead, m' was obtained for ten different $\{t\}_N$ sets for every point in Fig. 1. The values of m shown are the averages over the ten different sets of $\{t\}_N$. The error obtained, Δm, is fairly independent of βJ and βh, and, approximately, $\Delta m\approx 0.01$. Furthermore, $\Delta m \gg \delta m$ for every βJ and βh.

Two other sources of error, approximating a derivative by a finite difference [see Eqs. (4) and (5)], and the errors introduced by the computer when multiplying 4×10^3 matrices (12 digits were used by the computer to represent each real number), are negligible compared with Δm, or δm.

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[1]E. W. Montroll and G. S. Goel, Biopolymers 4, 855 (1966); A. A. Vedenov and A. M. Dykhne, Zh. Esp. Teor. Fiz. 55, 357 (1968) [Sov. Phys.-JETP 28, 187 (1969)].

[2]D. P. Landau and M. Blume, Phys. Rev. B 13, 287 (1976); to be able to read their figures correctly, see *ibid.* 16, (E)598 (1977).

[3]I owe this remark to D. Sherrington. See D. C. Rapaport, J. Phys. C 5, 1830 (1972).

[4]G. H. Wannier, *Statistical Physics* (Wiley, New York, 1966), p. 352.